

# Hamilton Operators, Discrete Symmetries, Brute Force and SymbolicC++

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**Abstract** To find the discrete symmetries of a Hamilton operator  $\hat{H}$  is of central importance in quantum theory. Here we describe and implement a brute force method to determine the discrete symmetries given by permutation matrices for Hamilton operators acting in a finite-dimensional Hilbert space. Spin and Fermi systems are considered as examples. A computer algebra implementation in SymbolicC++ is provided.

## 1 Introduction

In quantum mechanics the system is described by a self-adjoint (Hamilton) operator  $\hat{H}$  acting in a Hilbert space  $\mathcal{H}$ . Here we consider the finite dimensional Hilbert space  $\mathbb{C}^n$  where  $\hat{H}$  is a hermitian matrix [1, 2, 3, 4, 5]. One of the main tasks is to find the  $n \times n$  unitary matrices  $U$  such that  $U^* \hat{H} U = \hat{H}$ , where  $U^* = U^{-1}$ . The  $n \times n$  unitary matrices form the compact Lie group  $U(n)$ . Note that if  $U^* \hat{H} U = \hat{H}$  and  $V^* \hat{H} V = \hat{H}$  then  $(UV)^* \hat{H} (UV) = \hat{H}$ , where  $(UV)^* \equiv V^* U^*$ . Thus the set of matrices that keep  $\hat{H}$  invariant form a group themselves [6].

An important finite subgroup of the group  $U(n)$  are the  $n \times n$  permutation matrices. The number of  $n \times n$  permutation matrices is  $n!$ . For a given hermitian  $n \times n$  matrix  $\hat{H}$  we want to find all the  $n \times n$  permutation matrices  $P$  such that

$$P^T \hat{H} P = \hat{H}$$

where  $P^{-1} = P^T$ . These permutation matrices form a subgroup of all  $n \times n$  permutation matrices. Obviously the  $n \times n$  identity matrix  $I_n$  satisfies  $I_n \hat{H} I_n = \hat{H}$ .

Here we describe and implement in SymbolicC++ a brute force method to find these permutation matrices.

After this finite group has been found one determines the conjugacy classes. Now for a finite group  $G$  the number of conjugacy classes is equivalent to the number of non-equivalent irreducible matrix representations. From the conjugacy classes and the permutation matrices we can construct projection matrices to decompose the Hilbert space into invariant sub Hilbert spaces [6]. For example, if the permutation matrix  $P$  satisfies  $P^2 = I_n$ , then  $\Pi_1 = (I_n + P)/2$ ,  $\Pi_2 = (I_n - P)/2$  are projection matrices (with  $\Pi_1\Pi_2 = 0$ ) which can be utilized to decompose the Hilbert space  $\mathbb{C}^n$  into invariant subspaces.

## 2 Examples

We consider four examples: two Fermi systems and two spin systems.

Example 1. Let  $c_j^\dagger, c_j$  ( $j = 1, 2, 3$ ) be Fermi creation and annihilation operators, respectively. Consider the Hamilton operator

$$\hat{H} = t(c_1^\dagger c_2 + c_2^\dagger c_1 + c_2^\dagger c_3 + c_3^\dagger c_2 + c_1^\dagger c_3 + c_3^\dagger c_1) + k_1 c_1^\dagger c_1 + k_2 c_2^\dagger c_2 + k_3 c_3^\dagger c_3$$

and the number operator  $\hat{N} = c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3$ . Then  $[\hat{H}, \hat{N}] = 0$ . Since  $[\hat{H}, \hat{N}] = 0$  we find  $\hat{N}$  is a constant of motion, i.e. the total number of Fermi particles remains constant in the sense that if  $|n\rangle$  is an eigenstate of the number operator  $\hat{N}$  with eigenvalue  $n$  at time 0, then  $|n\rangle(t) = e^{-i\hat{H}t/\hbar}|n\rangle$  remains an eigenstate of  $\hat{N}$  with eigenvalue  $n$  for all times. Given a basis with two Fermi particles

$$c_1^\dagger c_2^\dagger |0\rangle, \quad c_1^\dagger c_3^\dagger |0\rangle, \quad c_2^\dagger c_3^\dagger |0\rangle.$$

Then we find the matrix representation of  $\hat{H}$

$$\hat{H} = \begin{pmatrix} k_1 + k_2 & t & -t \\ t & k_1 + k_3 & t \\ -t & t & k_2 + k_3 \end{pmatrix}.$$

The matrix representation of  $\hat{N}$  is the diagonal matrix  $2I_3$ , where  $I_3$  is the  $3 \times 3$  identity matrix. For  $k_1 \neq k_2, k_1 \neq k_3, k_2 \neq k_3$  no non-trivial symmetry is found. Also for  $k_1 \neq k_2, k_1 \neq k_3, k_2 = k_3$  no non-trivial symmetry is found. For  $k = k_1 = k_2 = k_3$  we obtain the permutation matrix

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

Thus using the projection matrices  $\Pi_1 = (I_3 - P)/2$ ,  $\Pi_2 = (I_3 - P)/2$  the Hilbert space  $\mathbb{C}^3$  can be decomposed into invariant subspaces. For the case  $k = k_1 = k_2 = k_3$  we find the eigenvalues  $2k - 2t$  and  $2k + t$  (twice).

Example 2. Consider the Hamilton operator (two-point Hubbard model)

$$\hat{H} = t(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

where  $n_{j\uparrow} := c_{j\uparrow}^\dagger c_{j\uparrow}$ ,  $n_{j\downarrow} := c_{j\downarrow}^\dagger c_{j\downarrow}$ . The operators  $c_{j\uparrow}^\dagger, c_{j\downarrow}^\dagger, c_{j\uparrow}, c_{j\downarrow}$  are Fermi operators. The Hubbard Hamilton operator commutes with the total number operator  $\hat{N}$  and the total spin operator  $\hat{S}_z$  where

$$\hat{N} := \sum_{j=1}^2 (c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow}), \quad \hat{S}_z := \frac{1}{2} \sum_{j=1}^2 (c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow}).$$

We consider the subspace with two particles  $N = 2$  and total spin  $S_z = 0$ . A basis in this four dimensional Hilbert space is given by

$$c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |\mathbf{0}\rangle, \quad c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |\mathbf{0}\rangle, \quad c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger |\mathbf{0}\rangle, \quad c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |\mathbf{0}\rangle.$$

We find the matrix representation of  $\hat{H}$  for this basis. Using the Fermi anti-commutation relations and  $c_{j\uparrow} |\mathbf{0}\rangle = 0$ ,  $c_{j\downarrow} |\mathbf{0}\rangle = 0$  for  $j = 1, 2$  we obtain the matrix representation of  $\hat{H}$  with the given basis

$$H = \begin{pmatrix} U & t & t & 0 \\ t & 0 & 0 & t \\ t & 0 & 0 & t \\ 0 & t & t & U \end{pmatrix}.$$

We find the four permutation matrices  $P_0 = I_4 = I_2 \star I_2 = I_2 \otimes I_2$ ,

$$P_1 = I_2 \star \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star I_2, \quad P_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where we define the star product  $\star$  of the two  $2 \times 2$  matrices  $A, B$  as [6]

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \star \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} := \begin{pmatrix} a_{11} & 0 & 0 & a_{12} \\ 0 & b_{11} & b_{12} & 0 \\ 0 & b_{21} & b_{22} & 0 \\ a_{21} & 0 & 0 & a_{22} \end{pmatrix}.$$

We note that the star product of two  $2 \times 2$  permutation matrices is a  $4 \times 4$  permutation matrix. Here  $P_1$  is the swap gate. The four permutation matrices  $P_0, P_1,$

$P_2, P_3$  form a commutative group with  $P_j^2 = I_4$  for  $j = 0, 1, 2, 3$ . If  $P$  is an  $n \times n$  permutation matrix with  $P^2 = I_n$  then

$$\Pi_1 = \frac{1}{2}(I_n + P), \quad \Pi_2 = \frac{1}{2}(I_n - P)$$

are projection matrices with  $\Pi_1 \Pi_2 = 0_n$ , where  $0_n$  is the  $n \times n$  zero matrix. Using the permutation matrices  $P_0$  and  $P_3$  (which form a subgroup) these projection operators can now be used to find the invariant subspaces

$$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \right\}, \quad \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \right\}.$$

These four vectors (after normalization) are known in quantum computing as the Bell basis [1, 2, 3, 4, 5]. This leads to the two invariant sub Hilbert spaces

$$\left\{ \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle + c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle), \quad \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle + c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle) \right\}$$

$$\left\{ \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle), \quad \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle) \right\}.$$

Example 3. Let  $\sigma_1, \sigma_2, \sigma_3$  be the Pauli spin matrices

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Consider the Hamilton operators [7]

$$\hat{H} = \hbar\omega_1 \sigma_3 \otimes I_2 + \hbar\omega_2 I_2 \otimes \sigma_1 + \epsilon(\sigma_3 \otimes \sigma_1)$$

$$\hat{K} = \hbar\omega_1 \sigma_3 \otimes I_2 + \hbar\omega_2 I_2 \otimes \sigma_1 + \epsilon(\sigma_1 \otimes \sigma_3)$$

where for the second Hamilton operator  $\hat{K}$  the interaction term is swapped around, i.e.  $\sigma_3 \otimes \sigma_1 \rightarrow \sigma_1 \otimes \sigma_3$ . This provides symmetry breaking. For the Hamilton operator  $\hat{H}$  we find the symmetries (permutation matrices)

$$P_0 = I_4, \quad P_1 = I_2 \oplus \sigma_1, \quad P_2 = \sigma_1 \oplus I_2, \quad P_3 = \sigma_1 \oplus \sigma_1$$

where  $\oplus$  denotes the direct sum. The four matrices form a commutative group under matrix multiplication. All satisfy  $P_j^2 = I_4$ . Thus we can use the projection

matrices  $\Pi_1 = (I_4 + P_j)/2$ ,  $\Pi_2 = (I_4 - P_j)/2$  to decompose the Hilbert space into two invariant subspaces. On the other hand for the Hamilton operator  $\hat{K}$  we only find the identity matrix  $P_0 = I_4$ , i.e. no non-trivial symmetry is admitted.

Example 4. Consider the Hamilton operator for triple spin interaction

$$\hat{H} = \sigma_1 \otimes \sigma_2 \otimes \sigma_3.$$

The eigenvalues of this hermitian and unitary  $8 \times 8$  matrix are  $+1$  (four-fold degenerate) and  $-1$  (four-fold degenerate). Owing to this degeneracy one expects a “large” number of symmetries. Applying the SymbolicC++ code we find 24 permutation matrices listed  $P_0, P_1, \dots, P_{23}$  with  $P_0 = I_8$ . They form a non-commutative group under matrix multiplication and are a subgroup of the group of  $8 \times 8$  permutation matrices. We note that the Kronecker product  $\otimes$  and the direct sum  $\oplus$  of two permutation matrices is again a permutation matrix [8]. Now we can list the ones with  $P_j^2 = I_8$ . We have

$$\begin{aligned} P_1 &= I_2 \oplus \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \oplus I_2 \\ P_2 &= (I_2 \star \sigma_1) \oplus (\sigma_1 \star I_2) \\ P_5 &= I_2 \otimes I_2 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \sigma_1 \otimes I_2 \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ P_6 &= (\sigma_1 \star I_2) \oplus (I_2 \star \sigma_1) \\ P_8 &= I_2 \otimes \sigma_1 \otimes \sigma_1 \\ P_{13} &= I_2 \otimes I_2 \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \sigma_1 \otimes I_2 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ P_{15} &= \sigma_1 \otimes I_2 \otimes I_2 \\ P_{23} &= \sigma_1 \otimes \sigma_1 \otimes \sigma_1. \end{aligned}$$

The other ones can be found by multiplication of these permutation matrices, for example  $P_3 = P_1 P_2$  etc. Thus the 24 matrices form a subgroup of the permutation group of  $8 \times 8$  matrices.

Another spin Hamilton operator studied is [9]

$$\hat{H} = a \sum_{j=1}^4 \sigma_3(j) \sigma_3(j+1) + b \sum_{j=1}^4 \sigma_1(j)$$

with cyclic boundary conditions, i.e.  $\sigma_3(5) \equiv \sigma_3(1)$ . Here  $a, b$  are real constants and  $\sigma_1, \sigma_2$  and  $\sigma_3$  are the Pauli matrices. Thus the underlying Hilbert space is

$\mathbb{C}^{16}$ . Recall that

$$\sigma_k(1) = \sigma_k \otimes I_2 \otimes I_2 \otimes I_2, \quad \sigma_k(2) = I_2 \otimes \sigma_k \otimes I_2 \otimes I_2$$

$$\sigma_k(3) = I_2 \otimes I_2 \otimes \sigma_k \otimes I_2, \quad \sigma_k(4) = I_2 \otimes I_2 \otimes I_2 \otimes \sigma_k$$

where  $k = 1, 2, 3$ . We obtain the symmetric  $16 \times 16$  matrix for  $\hat{H}$

$$\begin{pmatrix} 4a & b & b & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b & 0 & 0 & b & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 \\ b & 0 & 0 & b & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 \\ 0 & b & b & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\ b & 0 & 0 & 0 & 0 & b & b & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 \\ 0 & b & 0 & 0 & b & -4a & 0 & b & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & 0 & b & 0 & b & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & 0 & b & 0 & b & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b \\ b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b & b & 0 & b & 0 & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & b & 0 & b & 0 & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & b & 0 & -4a & b & 0 & 0 & b & 0 \\ 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & b & b & 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & b & b & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & b & 0 & 0 & b \\ 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & b & 0 & 0 & b \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & b & b & 4a \end{pmatrix}.$$

The Hamilton operator  $\hat{H}$  admits the  $C_{4v}$  symmetry group. The order of this non-commutative group is 8. One finds the following set of eight symmetries [9]

$$E : (1, 2, 3, 4) \rightarrow (1, 2, 3, 4) \quad C_2 : (1, 2, 3, 4) \rightarrow (3, 4, 1, 2)$$

$$C_4 : (1, 2, 3, 4) \rightarrow (2, 3, 4, 1) \quad C_4^3 : (1, 2, 3, 4) \rightarrow (4, 1, 2, 3)$$

$$\sigma_v : (1, 2, 3, 4) \rightarrow (2, 1, 4, 3) \quad \sigma'_v : (1, 2, 3, 4) \rightarrow (4, 3, 2, 1)$$

$$\sigma_d : (1, 2, 3, 4) \rightarrow (1, 4, 3, 2) \quad \sigma'_d : (1, 2, 3, 4) \rightarrow (3, 2, 1, 4)$$

which form a group isomorphic to  $C_{4v}$ . The symmetries can be found by calculating the  $16 \times 16$  permutation matrices such that  $\hat{H} = P^T \hat{H} P$ .

### 3 Code Description

Algorithms for finding all permutations of a sequence of objects are described by Knuth [10]. For a given  $n$  the permutation matrices are generated with the following algorithm. The algorithm implements the nested loops

```

For  $j_0 = 0, 1, \dots, n-1$  do
  For  $j_1 = 0, 1, \dots, n-1$  do
     $\vdots$ 
    For  $j_{n-1} = 0, 1, \dots, n-1$  do
      If  $j_0 \neq j_1 \neq \dots \neq j_{n-1}$  then
        use the permutation  $(0, 1, 2, \dots, n-1) \rightarrow (j_0, j_1, j_2, \dots, j_{n-1})$ .
      End loop
     $\vdots$ 
  End loop
End loop

```

**Algorithm to find all permutation matrices.**

1. Create an array  $(j_0, j_1, \dots, j_{n-1})$  of loop variables.
2. Initialize  $j_k := -1$  for  $k = 0, 1, \dots, n-1$ .
3. Initialize the loop variable index  $i$  to  $i := 0$ .
4. While  $i \geq 0$ 
  - (a) *Iterate.*  
Set  $j_i := j_i + 1$ .
  - (b) *Termination condition.*  
If  $j_i = n$  terminate this loop:
    - i. Set  $j_i := -1$ .
    - ii. *Exit the nested loop.*  
Set  $i := i - 1$ .
    - iii. Goto 4.
  - (c) If  $j_k = j_i$  for some  $k \in \{0, 1, \dots, i-1\}$  then goto 4.
  - (d) *Enter the next nested loop.*  
Set  $i := i + 1$ .
  - (e) *Innermost loop completes.*  
If  $i = n$  then use the permutation  $(0, 1, 2, \dots, n-1) \rightarrow (j_0, j_1, j_2, \dots, j_{n-1})$   
i.e. the permutation matrix  $P$  is given by

$$(P)_{uv} = \begin{cases} 1 & \text{if } v = j_u \\ 0 & \text{otherwise} \end{cases}.$$

The SymbolicC++ program [11] utilizes the vector class of the Standard Template Library. The Hamilton operator refers to example 2 in the text (two point Hubbard model).

```
// permutation.cpp

#include <iostream>
#include <vector>
#include "symbolicc++.h"
using namespace std;

int total;
Symbolic H;

void commutes(const Symbolic &P)
{
    if(P*H==H*P) cout << "P[" << total++ << "]" = " << P << endl;
}

void find_perm(int n,void (*use)(const Symbolic&))
{
    int i, k;
    Symbolic P;
    vector<int> j(n,-1);

    i = 0; j[0] = -1;
    while(i >= 0)
    {
        if(++j[i]==n) { j[i--] = -1; continue; }
        if(i < 0) break;
        for(k=0;k<i;++k) if(j[k]==j[i]) break;
        if(k!=i) continue;
        ++i;
        if(i==n)
        {
            P = 0*Symbolic("",n,n);
            for(k=0;k<n;k++) P(k,j[k]) = 1;
            use(P);
            --i;
        }
    }
}

int main(void)
{
    using SymbolicConstant::i;
    Symbolic sqrt2 = sqrt(Symbolic(2));
```



```

Symbolic U("U"); Symbolic t("t");
H = ((U,t,t,Symbolic(0)),(t,Symbolic(0),Symbolic(0),t),
      (t,Symbolic(0),Symbolic(0),t),(Symbolic(0),t,t,U));
cout << "H = " << H << endl;
total = 0;
find_perm(H.rows(),commutes);
return 0;
}

```

A Maxima implementation is available from the authors.

## 4 Conclusion

We applied a brute force method to find all possible permutation matrices that provide symmetries for given Hamilton operators in a finite dimensional Hilbert space. With growing size of the Hamilton operators matrix representation finding the permutation matrices becomes very time-consuming. A more efficient approach would be to find only the generators of the group of permutation matrices that provide symmetries for a given Hamilton operator. Another open question is how this method can be extended to find other classes of symmetries.

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